

PERFORMANCE ANALYSIS OF SOFT SENSING TECHNIQUE FOR A CONTINUOUS STIRRED TANK REACTOR

M.GEETHA

ICE Department, Peelamedu, Coimbatore, India

ABSTRACT

This paper deals with the implementation of a soft sensor technique namely Extended Kalman Filter (EKF) to estimate the state vectors of CSTR process using LabVIEW. The state variables considered are concentration and temperature of reactants in the reactor. An extensive simulation study has carried out to assess the performance of EKF under various operating conditions and model uncertainties.

KEYWORD: Soft Sensor Technique, EKF, CSTR, GRV, MSE, Lab VIEW

INTRODUCTION

In a plant, normally the different state measurements are done using hardware sensor devices. But it has inaccuracies due to different disturbances, ageing etc. Thus soft sensor techniques are used which are specifically named as state estimation techniques. Estimation is the determination of constants or variables for any system according to a performance level and based on the measurements taken from the process. It is an important pre-requisite for the safe and economical process operations in a plant analysis. Estimation of states of a Continuous Stirred Tank Reactor, which is highly non-linear is important for performance prediction, control application and simulation analysis. CSTR has wide applications in the field of petrochemical industries and biological processes. As the continuous measurement of reactant concentration and temperature in the reactor is difficult, estimation technique is used.

EKF, a modified version of Kalman filter is widely used to estimate the states of non-linear systems. EKF is extension to non-linear domain through local linearization. It is known for its high convergence rate, which improves the transient performance significantly. Additionally, accurate estimation and convergence in steady state requires high-frequency signals, which are also inherently met by EKFs with the measurement noises included in the model. Also, it gives better performance under different process uncertainties.

The use of LabVIEW for this work is to provide dataflow and graphical programming so that execution time is faster than other sequential programming tools. It has built-in functionality for simulation, data acquisition, instrument control, measurement analysis, and data presentation. The LabVIEW graphical development environment gives powerful tools to create applications without writing any lines of text-based code. The organization of the paper is as follows. Section II presents EKF algorithm. Section III describes the process considered for simulation study. Simulation results are presented in Section IV and conclusion in Section V.

EXTENDED KALMAN FILTER

The EKF implements a Kalman filter for a system dynamics that results from the linearization of the original non-linear filter dynamics around the previous state estimates. A vital operation performed in the Kalman filter is the propagation of a Gaussian Random Variable (GRV) through the system dynamics. In the EKF, the state distribution is approximated by a GRV, which is then propagated analytically through the first-order linearization of the nonlinear system.

The basic framework for the EKF involves estimation of the state of a discrete-time nonlinear dynamic system, described as

$$x_k = f(x_{k-1}, u_k, v_k) \quad (2.1)$$

$$y_k = h(x_k, n_k) \quad (2.2)$$

Where x_k is unobserved state of the system, x_{k-1} is the state estimate at time step k-1, u_k is input vector, y_k is observed signal. v_k and n_k are process and measurement noise which are assumed to be gaussian with zero mean having covariance Q_k and R_k respectively.

The nonlinear function $f()$ relates the state at time step k-1 to state at k. It can be used to compute the predicted state from the previous estimate. The function $h()$ relates the state at time step k to measurement at k. h can be used to compute the predicted measurement from the predicted state. However, f and h cannot be applied to the covariance directly. Instead a matrix of partial derivatives (the Jacobian) is computed. At each time step the Jacobian is evaluated with current predicted states.

The EKF has two distinct phases –Predict and Update. The predict phase uses the state estimate from the previous time step to produce an estimate of the state at the current time step. In the update phase, measurement information at the current time step is used to refine this prediction to arrive at a more accurate state estimate, again for the same current time step.

EKF algorithm is as follows.

Step 1: Time update equations

Predicted state:

$$\hat{x}_{k|k-1} = f(\hat{x}_{k-1|k-1}, u_k, 0) \quad (2.3)$$

Predicted estimate covariance:

$$P_{k|k-1} = F_k P_{k-1|k-1} F_k^T + Q_k \quad (2.4)$$

$$\text{Where } F_k = \left. \frac{\partial f}{\partial x} \right|_{\hat{x}_{k-1|k-1}, u_k} \quad (2.5)$$

Step 2: Measurement update equations

Innovation or measurement residual:

$$\tilde{z}_k = y_k - h(\hat{x}_{k|k-1}, 0) \quad (2.6)$$

Measurement covariance:

$$S_k = H_k P_{k|k-1} H_k^T + R_k \quad (2.7)$$

$$\text{Where } H_k = \left. \frac{\partial h}{\partial x} \right|_{\hat{x}_{k|k-1}} \quad (2.8)$$

Kalman gain:

$$K_k = P_{k|k-1} H_k^T S_k^{-1} \quad (2.9)$$

Updated state estimate:

$$\hat{x}_{k|k} = \hat{x}_{k|k-1} + K_k \tilde{z}_k \quad (2.10)$$

Updated covariance estimate:

$$P_{k|k} = (I - K_k H_k) P_{k|k-1} \quad (2.11)$$

MATHEMATICAL MODEL OF CSTR

A perfectly mixed CSTR is shown in figure 1

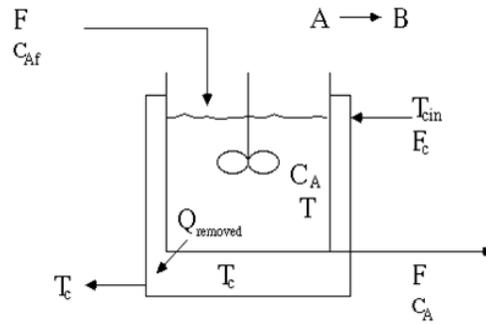


Fig. 1: CSTR

By applying material balance and energy balance equations, the resulting mathematical model equations are obtained as

$$\frac{dC_A}{dt} = \frac{F}{V} (C_{Af} - C_A) - r \quad (3.1)$$

$$\frac{dT}{dt} = \frac{F}{A} (T_f - T) + \left(\frac{-\Delta H}{\rho c_p} \right) r + \frac{\rho_c C_{pc}}{\rho C_p} q_c \left\{ 1 - \exp \left[\frac{-UA}{q_c \rho C_p} \right] \right\} (T_j - T) \quad (3.2)$$

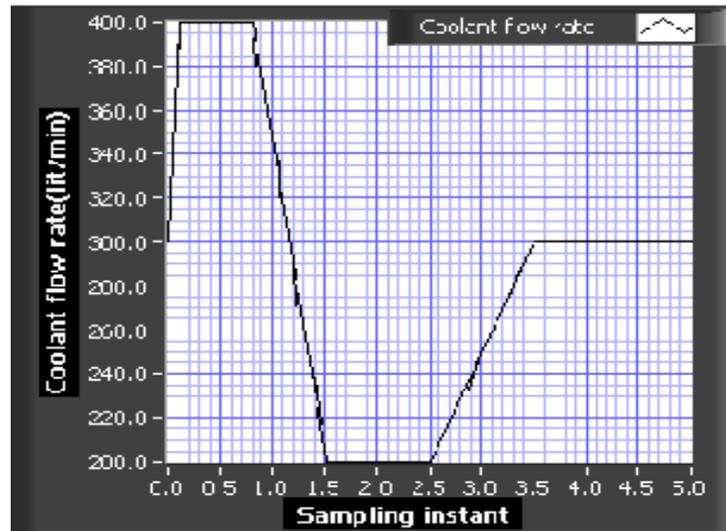
$$r = k_o \exp \left(\frac{-\Delta E}{RT} \right) C_A \quad (3.3)$$

The steady state operating data used for simulation study is given in table 1.

Table 1: Steady State Operating Data

Process variable	Normal operating condition
Measured product concentration(C_A)	0.877mol/lit
Reactor temperature (T)	324.475 K
Volumetric flow rate (F)	1000 lit/min
Reactor volume (V)	1000lit/min
Feed concentration (C_{Af})	1mol/lit
Feed temperature (Tf)	350K
Jacket temperature (T_j)	300K
Coolant flow rate(q_c)	300 lit/min
Heat of reaction (ΔH)	5e4 cal/mol
Reaction rate constant(k_0)	7.2e10 min ⁻¹
Activation energy term(ΔE)	1044 cal/mol
Ideal gas constant (R)	8.314 K
Liquid density(ρ, ρ_c)	1000 g/lit
Specific heat capacity (C_p, C_{pc})	0.239 cal/g.K

Both the temperature and concentration of CSTR are influenced by coolant flow rate. Figures 3 and 4 show the temperature and concentration responses of the CSTR for the coolant flow rate variation as shown in Figure2. From those responses, it can be concluded that the dynamic behaviour of the CSTR process is not the same at different operating points and the process is indeed non-linear [1].

**Fig. 2: Variation in Coolant Flow Rate**

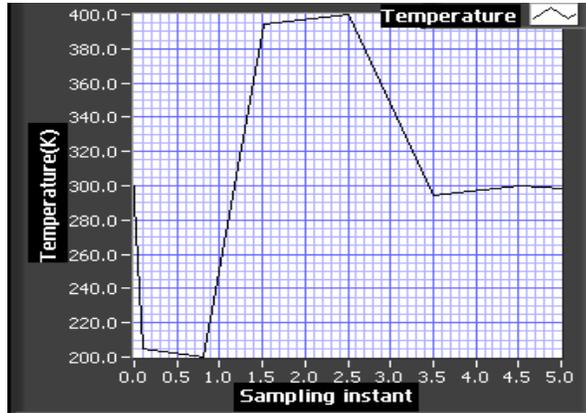


Fig. 3: Variation in Reactant Temperature

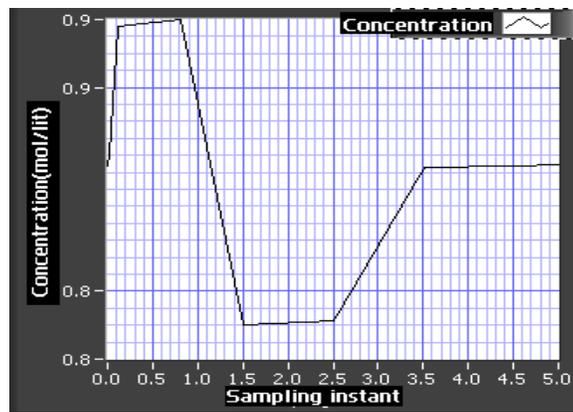


Fig. 4: Variation in Reactant Concentration

SIMULATION RESULTS AND ANALYSIS

In all the simulation studies, true state variables are computed by solving nonlinear differential equations using ODE solver in LabVIEW. These state variables are estimated using EKF algorithm assuming that the plant gets affected by gaussian noise. The resulting true and estimated values for both temperature and concentration under normal operating condition are shown in Figure 5 and Figure 6 respectively.

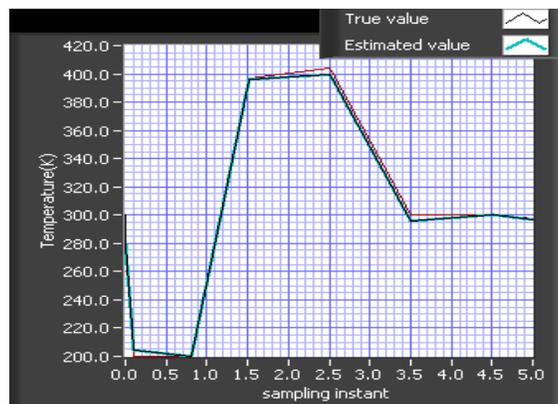


Fig.5: Evolution of True and Estimated Reactor Temperature with Varying Coolant Flow Rate

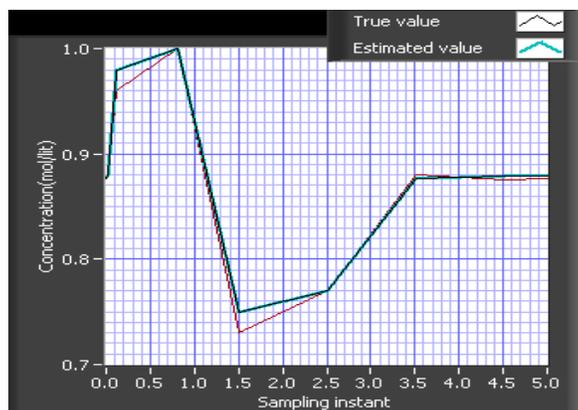


Fig.6: Evolution of True and Estimated Reactor Concentration with Varying Coolant Flow Rate

The performance of EKF was studied under following conditions and mean square error (MSE) was used as performance index.

I) Initial State Mismatch: Simulation studies are conducted with different initial state values and it is observed that the performance of the filters is affected mainly due to difference in initial values between process and model. Accordingly, simulations are carried out for different initial settings values for both temperature and concentration.

II) Model Parameter Mismatch: Due to inaccuracy in measurements and variation in operating conditions, parameters of process and model will not be identical and this may lead to poor estimation and hence control. Since the volumetric coolant flow rate affects both the temperature and concentration of the reactants simultaneously, it is chosen as the parameter to be mismatched between the model and process. Then estimation is carried out by giving up to 30% mismatch and the results are compared with by calculating mean square error. After 30%, it fails to converge.

III) Process Uncertainties: Studies are also made by assuming different levels of process noise for a fixed measurement error. Noises are introduced as standard deviation of 2 in the sampling instant 3 to Gaussian white noise. For a fixed value of Q and R, it is obtained that the EKF gives less estimation error.

Table 2: Comparison of MSE Values

Condition	MSE for Concentration	MSE for Temperature
Normal operation	0.0063	0.0048
Initial state mismatch	0.0296	0.0249
Model parameter mismatches (10%)	1.3131	2.4922
Model parameter mismatches (30%)	3.8106	4.0132
Process uncertainties	0.0052	0.0034

CONCLUSIONS

In this work a soft sensing technique namely Extended Kalman filter algorithm have been developed and implemented for the estimation of temperature and concentration in a CSTR plant using LabVIEW. At first, CSTR mathematical model was developed using mass and energy balance concepts. These states are first estimated using EKF under normal operating conditions. Then, simulation studies were conducted at different operating conditions such as initial state mismatch, model parameter mismatch and different process uncertainties. The result show that for most of the

operating conditions, where the change is not large enough, EKF is found to be better and convergence is faster. When there is a large difference in parameters between actual process and model, performance of EKF is not satisfactory. It gives better performance when there are large process uncertainties.

REFERENCES

1. K. Srinivasan, J. Prakash, "Non-linear State Estimation for Continuous Stirred Tank Reactor using Neural Network State Filter", IEEE annual conference, 2006
2. M.Kodabandeh, H. Bolandi, "Model predictive control with State Estimation and Adaptation Mechanism for a Continuous Stirred Tank Reactor," International Conference on Control, Automation and Systems, pp. 1466-1471, October, 2007.
3. S. Mohammadi, H. Keivani, "Using Sequential Kalman Filters for State Estimation of Nonlinear Systems", Proceedings of the 26th Chinese Control Conference, July, 2007.
4. U. Sabura Banu, G Uma, "Modelling of CSTR by fuzzy clustering", Proceedings of India International Conference on Power Electronics, pp 371-376, 2006.
5. Ehsan Moshksar, Faridoun Shabaninia, "Fuzzy Sliding Mode Control Algorithm and Extended Kalman Filter for Nonlinear Chemical Reactors", International conference on Information recursion and integration, pp 322-325, August, 2010.
6. Vahid Fathabadi, Mehdi Shahbazian, "Performance Monitoring of a CSTR Plant Using Asynchronous Data Fusion Based on Extended Kalman Filter", International Conference on Emerging Technologies, pp. 118-123, August, 2009.
7. U. Sabura Banu, G Uma, "Modelling of CSTR by fuzzy clustering", Proceedings of India International Conference on Power Electronics, pp 371-376, 2006
8. Jiri Vojtesek, Petr Dostal, "simulation analyses of continuous stirred tank reactor", IEEE transactions, Vol 24, pp 27-31, December, 2008
9. Fei Zhang, Guangjun Liu, "A Battery State of Charge Estimation Method with Extended Kalman Filter", IEEE International Conference on Advanced Intelligent Mechatronics, July 2008. A. Soukkou, A. Khellaf, "Optimal control of a CSTR process", Brazilian journal of chemical engineering, Vol. 25, pp. 799-812, December, 2008

